



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 27, 2025 – 11:29 AM EDT

PDB ID : 7I2F
Title : Group deposition for crystallographic fragment screening of the NS5 RNA-dependent RNA polymerase from Dengue virus serotype 2 – Crystal structure of the NS5 RNA-dependent RNA polymerase from Dengue virus serotype 2 in complex with Z1079168976 (DENV2_NS5A-x0378)
Authors : Aschenbrenner, J.C.; Saini, M.; Chopra, A.; Marples, P.G.; Balcomb, B.H.; Lithgo, R.M.; Fearon, D.; von Delft, F.; Ruiz, F.X.; Arnold, E.
Deposited on : 2025-03-06
Resolution : 2.05 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)

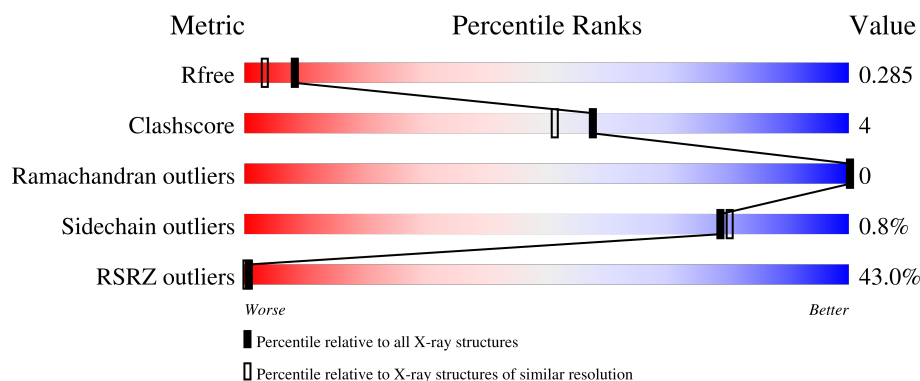
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.05 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	2096 (2.04-2.04)
Clashscore	180529	2229 (2.04-2.04)
Ramachandran outliers	177936	2217 (2.04-2.04)
Sidechain outliers	177891	2217 (2.04-2.04)
RSRZ outliers	164620	2096 (2.04-2.04)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	637	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
 Validation Pipeline (wwPDB-VP) : 2.41.4

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	PO4	A	1007	-	-	X	-

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 5086 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called NS5 RNA-dependent RNA polymerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	563	Total	C	N	O	S	0	6	0
			4660	2936	833	857	34			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	264	GLY	-	expression tag	UNP Q91H74
A	265	PRO	-	expression tag	UNP Q91H74

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Zn	0	0
			2	2		

- Molecule 3 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: C₆H₁₃NO₄S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	1
			24	12	2	8	2		

- Molecule 4 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C_2H_6OS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	O	S	0	0
			4	2	1	1		
4	A	1	Total	C	O	S	0	0
			4	2	1	1		
4	A	1	Total	C	O	S	0	0
			4	2	1	1		

- Molecule 5 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	P	0	0
			5	4	1		
5	A	1	Total	O	P	0	0
			5	4	1		

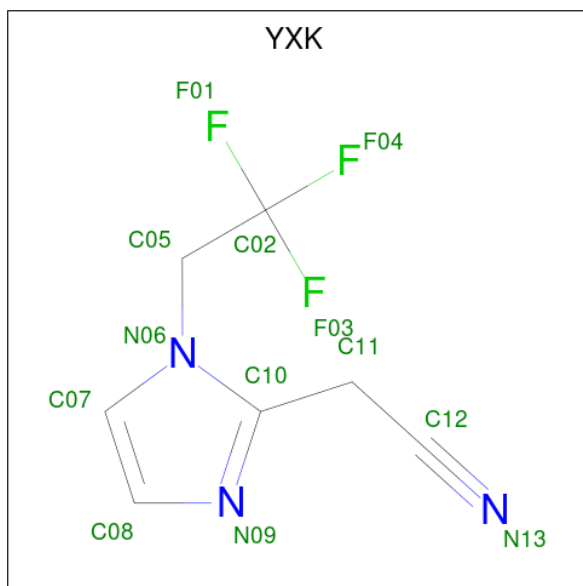
- Molecule 6 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			7	4	3		

- Molecule 7 is [1-(2,2,2-trifluoroethyl)-1H-imidazol-2-yl]acetonitrile (three-letter code: YXK)

(formula: $C_7H_6F_3N_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	F	N	0	0
			13	7	3	3		

- Molecule 8 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	1	Total	Cl	0	0
			1	1		

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	357	Total	O	0	0
			357	357		

4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	82.38Å 115.78Å 147.97Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.59 – 2.05 45.59 – 2.05	Depositor EDS
% Data completeness (in resolution range)	99.7 (45.59-2.05) 99.7 (45.59-2.05)	Depositor EDS
R_{merge}	0.38	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.07 (at 2.05Å)	Xtriage
Refinement program	REFMAC 5.8.0267, REFMAC5	Depositor
R, R_{free}	0.193 , 0.251 0.263 , 0.285	Depositor DCC
R_{free} test set	2262 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	37.2	Xtriage
Anisotropy	0.232	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 137.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	5086	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.66% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PEG, DMS, ZN, YXK, CL, MES, PO4

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.72	1/4764 (0.0%)	0.82	1/6423 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	510	GLU	CD-OE2	5.80	1.32	1.25

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	815	ARG	NE-CZ-NH2	-5.58	117.51	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4660	0	4562	38	0
2	A	2	0	0	0	0
3	A	24	0	26	1	0
4	A	12	0	18	3	0
5	A	10	0	0	3	0
6	A	7	0	10	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	13	0	0	0	0
8	A	1	0	0	0	0
9	A	357	0	0	8	2
All	All	5086	0	4616	41	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (41) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:664:ASP:OD1	5:A:1007:PO4:O4	1.81	0.97
1:A:513:HIS:HA	9:A:1101:HOH:O	1.89	0.71
1:A:653:GLU:O	1:A:656:SER:OG	2.09	0.70
1:A:400:THR:HA	1:A:426:VAL:HG21	1.74	0.69
1:A:733:GLU:O	1:A:737:ARG:HG3	1.92	0.69
1:A:649:ARG:HG3	1:A:650:VAL:HG13	1.74	0.69
1:A:274:LEU:HA	1:A:277:ILE:HG12	1.75	0.68
4:A:1004:DMS:H11	9:A:1278:HOH:O	1.93	0.68
1:A:835:GLU:O	9:A:1102:HOH:O	2.12	0.66
1:A:453:ASN:ND2	1:A:579:ARG:HD2	2.17	0.59
1:A:513:HIS:CA	9:A:1101:HOH:O	2.47	0.58
1:A:510:GLU:O	1:A:514:LYS:HG3	2.04	0.56
1:A:303:TRP:CE3	1:A:593:ILE:HD12	2.41	0.56
1:A:790:THR:HG21	9:A:1419:HOH:O	2.07	0.54
1:A:429:SER:O	1:A:433:GLU:HG3	2.08	0.54
1:A:664:ASP:OD1	5:A:1007:PO4:P	2.65	0.53
1:A:430:GLY:O	1:A:434:LEU:HG	2.10	0.52
1:A:375:LYS:HD2	1:A:549:ASN:OD1	2.10	0.52
1:A:562:LYS:HE3	1:A:566:GLU:OE2	2.11	0.51
1:A:887:LYS:HG3	1:A:890:ARG:NH2	2.26	0.51
4:A:1004:DMS:C1	9:A:1278:HOH:O	2.56	0.49
1:A:438:GLU:HG3	1:A:449:THR:OG1	2.13	0.49
4:A:1004:DMS:H12	9:A:1263:HOH:O	2.12	0.49
1:A:274:LEU:HA	1:A:277:ILE:CG1	2.43	0.49
1:A:541:ARG:HD2	1:A:685:GLY:O	2.14	0.48
1:A:748:LEU:HD13	3:A:1003[A]:MES:H61	1.97	0.47
1:A:447:CYS:SG	1:A:450:CYS:HB2	2.55	0.47
1:A:337:MET:HG2	9:A:1344:HOH:O	2.14	0.46
1:A:534:ASP:OD1	5:A:1007:PO4:O4	2.33	0.46
1:A:303:TRP:CD2	1:A:593:ILE:HD12	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:390:THR:HG22	1:A:391:PRO:O	2.17	0.45
1:A:503:SER:O	1:A:504:LEU:HB2	2.17	0.45
1:A:635:LEU:HG	1:A:639:GLU:HB3	1.99	0.45
1:A:420:LYS:HB3	1:A:424:GLU:OE2	2.17	0.44
1:A:452:TYR:O	1:A:578:VAL:HA	2.18	0.43
1:A:599:ARG:HG2	1:A:606:THR:HG23	2.01	0.42
1:A:402:LYS:NZ	1:A:494:GLU:OE2	2.42	0.42
1:A:311:THR:HG21	1:A:590:MET:HB2	2.01	0.42
1:A:321:VAL:HG11	1:A:326:ARG:CZ	2.50	0.42
1:A:889:PHE:O	1:A:891:ARG:N	2.52	0.41
1:A:273:ASN:N	1:A:275:ASP:OD1	2.54	0.41

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:1126:HOH:O	9:A:1126:HOH:O[2_445]	1.88	0.32
9:A:1299:HOH:O	9:A:1381:HOH:O[2_545]	1.99	0.21

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	555/637 (87%)	534 (96%)	21 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	502/554 (91%)	498 (99%)	4 (1%)	79	80

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	426	VAL
1	A	570	LYS
1	A	580	VAL
1	A	717	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	786	HIS
1	A	862	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 3 are monoatomic - leaving 9 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	PEG	A	1009	-	6,6,6	0.18	0	5,5,5	0.06	0
3	MES	A	1003[A]	-	12,12,12	0.85	0	15,16,16	0.48	0
5	PO4	A	1007	-	4,4,4	3.19	2 (50%)	6,6,6	0.67	0
4	DMS	A	1004	-	3,3,3	0.38	0	3,3,3	0.32	0
5	PO4	A	1008	-	4,4,4	1.24	1 (25%)	6,6,6	0.40	0
3	MES	A	1003[B]	-	12,12,12	1.05	0	15,16,16	0.46	0
4	DMS	A	1005	-	3,3,3	0.21	0	3,3,3	0.05	0
4	DMS	A	1006	-	3,3,3	0.14	0	3,3,3	0.30	0
7	YXK	A	1010	-	12,13,13	0.49	0	11,18,18	0.44	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	MES	A	1003[B]	-	-	5/6/14/14	0/1/1/1
6	PEG	A	1009	-	-	2/4/4/4	-
3	MES	A	1003[A]	-	-	2/6/14/14	0/1/1/1
7	YXK	A	1010	-	-	0/5/8/8	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1007	PO4	P-O1	5.59	1.63	1.50
5	A	1008	PO4	P-O1	2.46	1.56	1.50
5	A	1007	PO4	P-O4	-2.25	1.48	1.54

There are no bond angle outliers.

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1003[B]	MES	C8-C7-N4-C3
3	A	1003[B]	MES	C7-C8-S-O2S
3	A	1003[B]	MES	C7-C8-S-O3S
6	A	1009	PEG	O2-C3-C4-O4

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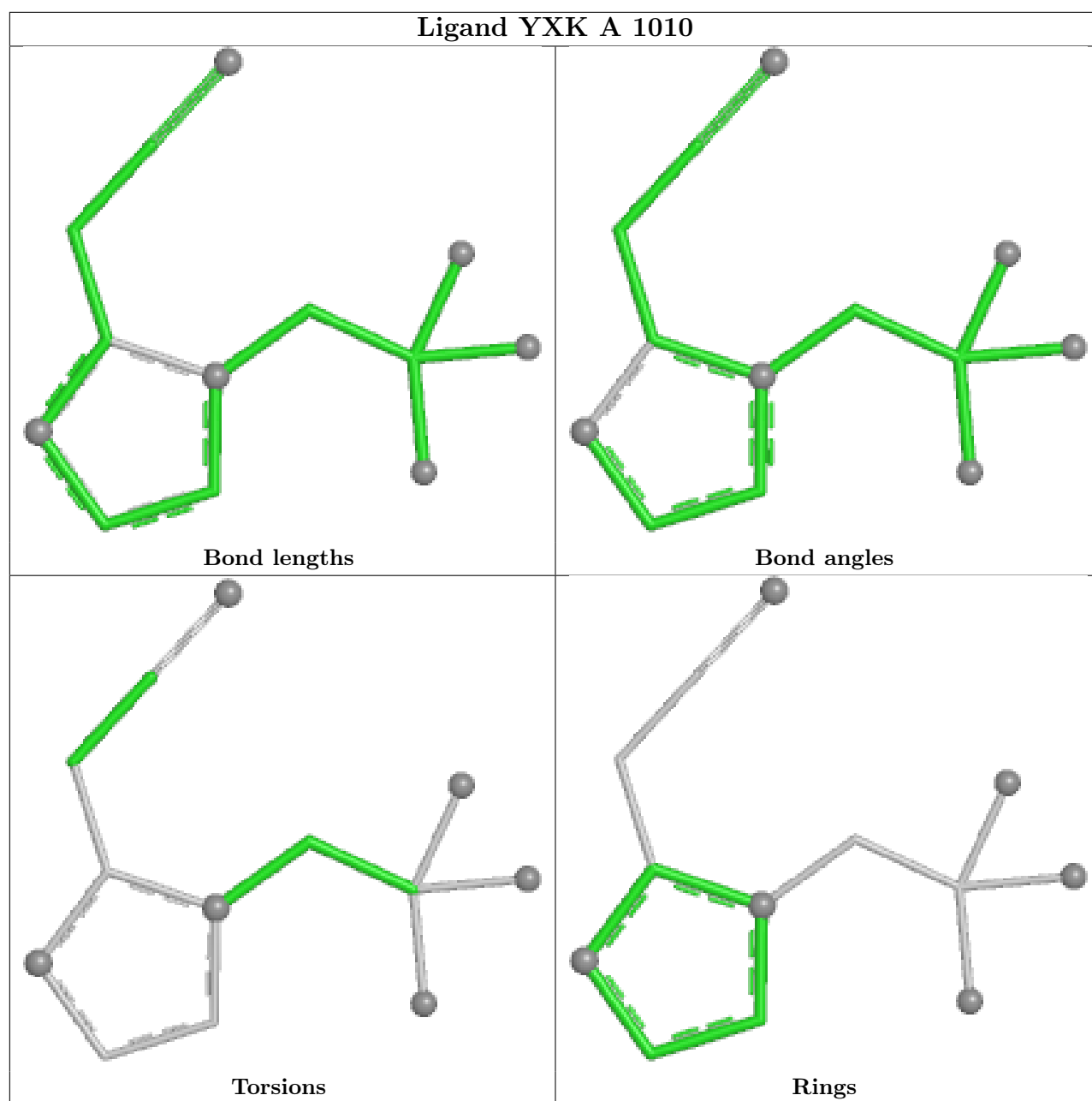
Mol	Chain	Res	Type	Atoms
3	A	1003[B]	MES	C8-C7-N4-C5
3	A	1003[B]	MES	C7-C8-S-O1S
3	A	1003[A]	MES	C8-C7-N4-C5
6	A	1009	PEG	C4-C3-O2-C2
3	A	1003[A]	MES	C8-C7-N4-C3

There are no ring outliers.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1003[A]	MES	1	0
5	A	1007	PO4	3	0
4	A	1004	DMS	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	563/637 (88%)	3.41	242 (42%) 1 0	7, 38, 87, 125	122 (21%)

All (242) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	538	TRP	18.8
1	A	432	TRP	18.6
1	A	632	ILE	18.4
1	A	475	TRP	17.4
1	A	399	PHE	17.4
1	A	478	TRP	16.6
1	A	359	VAL	16.5
1	A	536	ALA	16.5
1	A	483	PHE	16.5
1	A	435	VAL	16.4
1	A	484	LEU	16.2
1	A	631	SER	15.7
1	A	372	LYS	15.6
1	A	426	VAL	15.2
1	A	476	TYR	15.1
1	A	534	ASP	15.0
1	A	535	THR	14.9
1	A	367	LYS	14.7
1	A	431	PHE	14.6
1	A	434	LEU	14.5
1	A	361	THR	14.3
1	A	400	THR	14.1
1	A	425	ALA	14.0
1	A	360	ASP	13.9
1	A	598	GLN	13.7
1	A	801	HIS	13.6
1	A	430	GLY	13.6

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Mol	Chain	Res	Type	RSRZ
1	A	537	GLY	13.6
1	A	597	ASP	13.4
1	A	539	ASP	13.3
1	A	474	ILE	13.2
1	A	403	VAL	13.1
1	A	477	MET	13.0
1	A	634	HIS	12.9
1	A	693	GLN	12.7
1	A	436	ASP	12.4
1	A	479	LEU	12.2
1	A	402	LYS	12.0
1	A	630	LYS	11.8
1	A	747	SER	11.8
1	A	365	GLU	11.6
1	A	429	SER	11.6
1	A	421	SER	11.5
1	A	437	LYS	11.4
1	A	358	LYS	11.2
1	A	368	GLU	11.1
1	A	748	LEU	11.1
1	A	294	TYR	11.0
1	A	596	ARG	10.9
1	A	741[A]	SER	10.9
1	A	363	THR	10.7
1	A	690	ASP	10.6
1	A	719[A]	LYS	10.5
1	A	401	ARG	10.5
1	A	482	ARG	10.4
1	A	419	TRP	10.3
1	A	473	ALA	10.3
1	A	292	TRP	10.2
1	A	746	TRP	10.2
1	A	428	ASP	10.2
1	A	424	GLU	10.2
1	A	839	LEU	10.1
1	A	648	VAL	10.1
1	A	405	SER	10.0
1	A	518	ILE	10.0
1	A	293	HIS	10.0
1	A	311	THR	9.8
1	A	752	ALA	9.7
1	A	749	ARG	9.6

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Mol	Chain	Res	Type	RSRZ
1	A	763[A]	SER	9.5
1	A	512[A]	LEU	9.5
1	A	588	THR	9.4
1	A	753	CYS	9.4
1	A	404	ARG	9.3
1	A	727	PRO	9.2
1	A	754	LEU	9.1
1	A	406	ASN	9.1
1	A	505	SER	9.1
1	A	433	GLU	9.0
1	A	742	GLN	9.0
1	A	744	ALA	8.9
1	A	656	SER	8.8
1	A	427	GLU	8.8
1	A	657	ARG	8.7
1	A	498	PHE	8.6
1	A	423	ARG	8.4
1	A	277	ILE	8.4
1	A	504	LEU	8.3
1	A	499	SER	8.2
1	A	713	PHE	8.1
1	A	705	GLN	8.1
1	A	649	ARG	8.1
1	A	864[A]	GLN	8.0
1	A	785[A]	SER	8.0
1	A	357	GLU	8.0
1	A	420	LYS	7.7
1	A	720	ASP	7.7
1	A	658	MET	7.6
1	A	288	HIS	7.5
1	A	718	MET	7.5
1	A	751	THR	7.4
1	A	790	THR	7.3
1	A	364	GLN	7.2
1	A	581	GLN	7.0
1	A	887	LYS	7.0
1	A	500	ARG	7.0
1	A	856	ARG	7.0
1	A	835	GLU	7.0
1	A	312	LYS	6.9
1	A	295	ASP	6.9
1	A	583	PRO	6.9

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Mol	Chain	Res	Type	RSRZ
1	A	843	GLU	6.9
1	A	670	LEU	6.8
1	A	291	SER	6.5
1	A	513	HIS	6.5
1	A	298	HIS	6.4
1	A	653	GLU	6.4
1	A	503	SER	6.3
1	A	600	GLY	6.2
1	A	290	THR	6.2
1	A	750	GLU	6.2
1	A	418	LYS	6.1
1	A	297	ASP	6.1
1	A	551	GLU	6.0
1	A	770	ARG	5.8
1	A	568	ILE	5.5
1	A	286	GLN	5.5
1	A	745	GLY	5.5
1	A	289	GLU	5.3
1	A	888	ARG	5.3
1	A	422	ALA	5.2
1	A	791	SER	5.1
1	A	502	ASN	5.1
1	A	589	VAL	5.1
1	A	800	THR	5.1
1	A	274	LEU	5.0
1	A	301	LYS	5.0
1	A	582	ARG	4.9
1	A	281	ILE	4.9
1	A	302	THR	4.7
1	A	273	ASN	4.6
1	A	635	LEU	4.6
1	A	393	MET	4.6
1	A	275	ASP	4.6
1	A	441	LEU	4.6
1	A	544	LEU	4.5
1	A	278	GLY	4.4
1	A	676	SER	4.4
1	A	309	TYR	4.3
1	A	319	SER	4.3
1	A	300	TYR	4.2
1	A	439	ARG	4.2
1	A	743	GLY	4.2

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Mol	Chain	Res	Type	RSRZ
1	A	296	GLN	4.2
1	A	818	ILE	4.2
1	A	287	GLU	4.2
1	A	396	ARG	4.0
1	A	276	ILE	3.9
1	A	569	PHE	3.9
1	A	308	SER	3.9
1	A	305	TYR	3.9
1	A	454	MET	3.9
1	A	501	GLU	3.9
1	A	343	MET	3.9
1	A	694	TRP	3.8
1	A	481	ALA	3.8
1	A	299	PRO	3.8
1	A	366	PRO	3.8
1	A	284	ILE	3.7
1	A	584	THR	3.7
1	A	306	HIS	3.6
1	A	593	ILE	3.5
1	A	455	MET	3.5
1	A	453	ASN	3.4
1	A	489	LEU	3.4
1	A	799	ALA	3.4
1	A	444	GLU	3.4
1	A	638	THR	3.3
1	A	279	LYS	3.3
1	A	590	MET	3.3
1	A	891	ARG	3.3
1	A	344	THR	3.3
1	A	452	TYR	3.2
1	A	880	THR	3.2
1	A	558	GLU	3.2
1	A	878	GLU	3.2
1	A	637	VAL	3.1
1	A	680	ALA	3.0
1	A	480	GLY	3.0
1	A	645	ASN	2.9
1	A	440	ASN	2.9
1	A	622	GLN	2.8
1	A	560	GLU	2.8
1	A	570	LYS	2.8
1	A	886	MET	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	448	GLU	2.8
1	A	304	ALA	2.7
1	A	545	GLU	2.7
1	A	869	GLN	2.7
1	A	303	TRP	2.7
1	A	566	GLU	2.7
1	A	882	TYR	2.6
1	A	556	HIS	2.6
1	A	375	LYS	2.6
1	A	572	THR	2.6
1	A	883	MET	2.6
1	A	362	ARG	2.6
1	A	397	GLU	2.6
1	A	451	VAL	2.6
1	A	644	LYS	2.5
1	A	677	ALA	2.5
1	A	889	PHE	2.5
1	A	495	ASP	2.5
1	A	679	THR	2.5
1	A	564	LEU	2.4
1	A	830	VAL	2.4
1	A	652	ARG	2.4
1	A	881	ASP	2.4
1	A	603	GLN	2.4
1	A	789	PRO	2.3
1	A	540	THR	2.3
1	A	819	GLN	2.3
1	A	282	GLU	2.3
1	A	370	THR	2.3
1	A	699	GLY	2.2
1	A	577	VAL	2.2
1	A	580	VAL	2.2
1	A	820	GLU	2.2
1	A	576	LYS	2.2
1	A	376	ILE	2.2
1	A	487	GLU	2.2
1	A	285	LYS	2.1
1	A	642	ALA	2.1
1	A	592	ILE	2.1
1	A	834	GLU	2.1
1	A	280	ARG	2.1
1	A	764	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	804	MET	2.1
1	A	876	ASN	2.0
1	A	641	ILE	2.0
1	A	578	VAL	2.0
1	A	337	MET	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

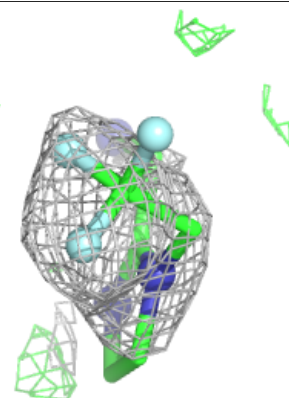
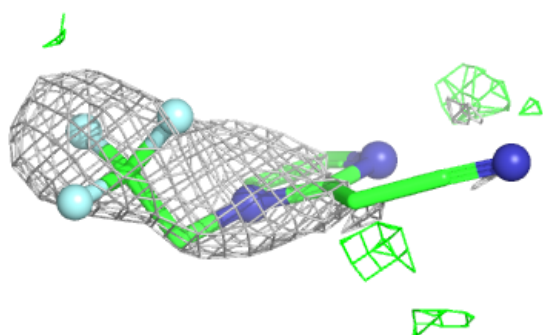
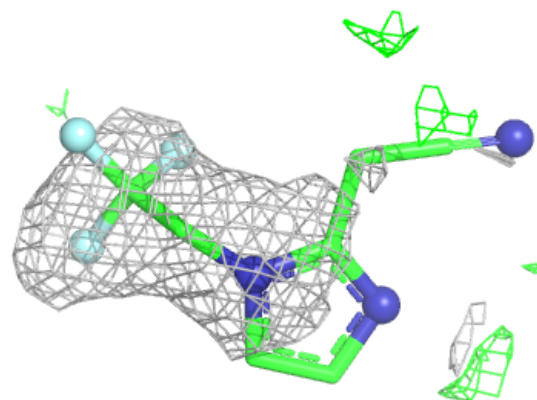
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	PO4	A	1008	5/5	0.63	0.19	80,85,100,116	0
7	YXK	A	1010	13/13	0.71	0.30	21,25,29,30	13
6	PEG	A	1009	7/7	0.80	0.18	67,74,79,81	0
5	PO4	A	1007	5/5	0.81	0.18	43,48,57,73	0
4	DMS	A	1005	4/4	0.87	0.20	91,92,93,100	0
4	DMS	A	1004	4/4	0.93	0.15	51,52,54,55	0
3	MES	A	1003[B]	12/12	0.94	0.41	876,889,933,935	12
4	DMS	A	1006	4/4	0.94	0.24	57,58,58,59	0
3	MES	A	1003[A]	12/12	0.94	0.41	32,35,37,37	12
2	ZN	A	1002	1/1	0.99	0.03	57,57,57,57	0
8	CL	A	1011	1/1	0.99	0.04	43,43,43,43	0
2	ZN	A	1001	1/1	1.00	0.01	27,27,27,27	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around YXK A 1010:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers ⓘ

There are no such residues in this entry.